Mathematics, Hybrid computing and HPC

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Mathematics, Hybrid computing and HPC

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HPC appears more and more as a key player in the field of numerical simulation and data processing. This trend comes of course with the desire to perform simulations that are closer and closer to real world situations, and with the development of clusters and platforms that provide access to hundreds to thousands CPU/GPU nodes.

The application domains encompass many fields, from fluid mechanics to biology and nano-sciences, in academic research as well as for industrial applications.

Concerning industrial applications, major groups have often already a good practice of HPC, with dedicated manpower and available in-house platforms. The access of SMEs to HPC is more problematic as they do not have the appropriate resources in hardware and manpower, and it is sometimes hard for them to have a clear idea of the gain they will obtain through HPC. In the first part of the talk, I will talk about a national initiative led by INRIA, GENCI and BPI, to promote the access of SMEs to HPC. This initiative provides support both in terms of market analysis, access to hardware and technical environment. It now involves middle-size HPC platforms that are distributed in French universities. This initiative will therefore give new opportunities to researchers, in particular mathematicians, to be connected to industrial collaborations.

HPC is actually not only a question of accessing hardware and adapting existing codes to massively parallel platforms. It also raises questions about mathematical and numerical models that optimize the emerging hardware and analyze the huge amount of data associated with these simulations, and software engineering to distribute algorithms on heterogeneous clusters. Mathematicians therefore can use HPC as a mean to access challenging industrial collaborations in which they can contribute through new methods and algorithms, in both scientific computing and statistics.

In the second part of the talk I will try to illustrate this point of view with ongoing research in Grenoble related to High Performance (hybrid) Computing for the direct numerical simulation of turbulent mixing. Turbulent mixing appears in many applications (environment, combustion, ..). The turbulent mixing of a scalar often induces a separation of the scales that appear in the flow and in the scalar. This feature makes turbulent mixing a natural candidate for hybrid computation, where difference computed quantities, the flow and the scalar in this example, are treated by different algorithms and, ultimately, distributed to different type of hardwares. We will describe such an hybrid approach, combining a spectral flow solver and a semi-lagrangian scalar solver, and running on massively parallel platforms. We will show how this numerical approach allows to capture the scalar up to the dissipative scales at a minimal cost.

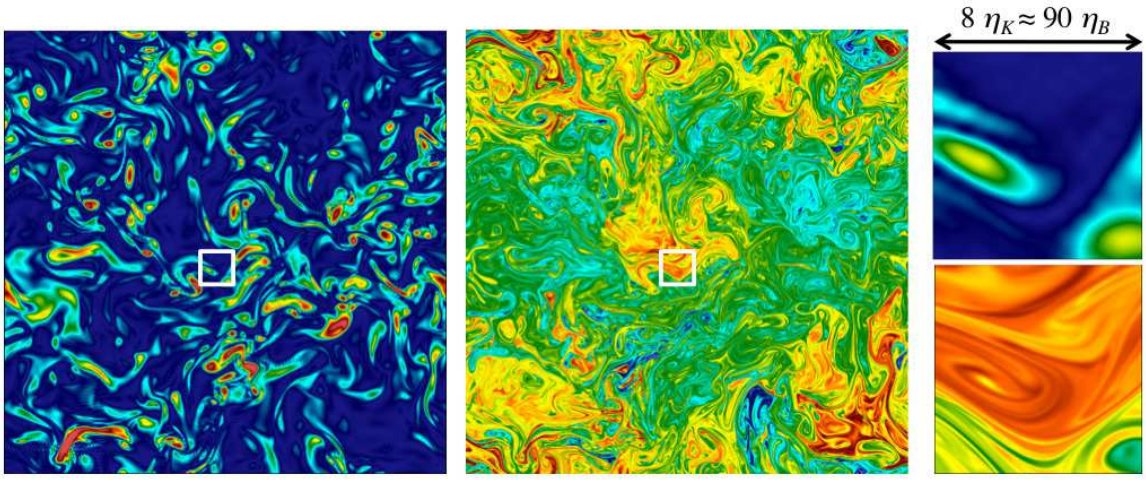

FIGURE 1. Vorticity (left) and scalar (middle) scales in a turbulent flow. Schmidt number=128. Right pictures : zoom of flow and scalar showing the scale gap between the vorticity (top) and the scalar (bottom).